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Our accomplishments for the period of 15 December 97 - 14 December 00 can be summarized in five key areas. They are:

A. Morphology evolution of ion-irradiated Au(111);
B. Thermal relaxation of a sputter-roughened surface;
C. Energetic deposition of Cu on Cu(111);
D. Monte Carlo and Molecular Dynamics simulations of mound formation, thermal relaxation, and energetic deposition; and
E. Hardware development for studies of energetic deposition with controlled energy beams.

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FINAL REPORT

GRANT NO. F49620-97-1-0020

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REPORT PERIOD: 15 DEC 96 - 14 DEC 00

PROJECT TITLE: FUNDAMENTALS OF METAL THIN FILM DEPOSITION AND SURFACE PROCESSING WITH HYPERTHERMAL IONS

1) OBJECTIVES

Our objectives are to understand the microscopic processes that occur during thin film growth and surface processing with energetic beams, and to determine how and why the use of energetic beams influences macroscopic film and surface properties. Technologically important growth techniques (e.g., sputter and plasma deposition, ion-assisted deposition, pulsed laser deposition) employ hyperthermal energy (a few eV to several hundred eV) particles, resulting in lower growth temperatures and films with substantially different properties than thermally deposited films [1]. These differences result in part from the highly non-equilibrium atomic motions that can occur when energy is transferred to the surface atoms by the collisions of the hyperthermal incident particles [2]. In addition, the hyperthermal beams used routinely in surface processing techniques, such as sputter cleaning, patterning, and depth profiling, can give rise to a variety of surface morphologies [3]. It is thus desirable to gain a better understanding of the microscopic processes that occur during energetic beam thin film growth and surface processing and how they influence surface properties.

We are using the complementary techniques of real-time X-ray diffraction and Scanning Tunneling Microscopy (STM) to study surface morphology evolution during growth and sputtering with energetic beams. The combined use of X-rays and STM provides a more complete picture than either technique alone. X-rays measure the long range and average properties of the surface, and are ideally suited to real-time observations. STM provides real-space measurements of surface structure down to the atomic scale. The experiments are combined with state-of-the-art simulations to better understand how microscopic processes influence macroscopic properties. Specific areas of investigation include:

Surface Processing with Ion Beams:

We have studied how surface morphology evolves during ion beam erosion (or sputtering) of a metal surface. Depending on beam and substrate conditions, we observe a variety of behaviors, including the production of smooth, mounded, and rippled morphologies. The different morphologies and the time-evolution of the surface features give information about the microscopic mechanisms that govern mass transport on the surface. Some of this information is extracted from Monte Carlo simulations that we have used to relate microscopic processes to macroscopic properties. (See Section 2 – Accomplishments/New Findings).

Specifically, we have studied morphology evolution of the Au(111) surface during Ar^+ ion irradiation using real-time X-ray scattering at the Cornell High Energy Synchrotron Source (CHESS), and separately using STM. Erosion occurs by different mechanisms depending on the surface temperature: step retraction at high temperatures, layer-by-layer removal at intermediate temperatures, and three-dimensional pattern formation at low temperatures. In the low temperature regime a pattern of pits and

mounds forms. We have made the first real-time measurement of the time-dependence of the characteristic spacing between these features. X-ray studies indicate the feature spacing follows a power law in time with an exponent of 0.27 [4]. This exponent is consistent with the existence of barriers for interlayer transport of adatoms and/or vacancies in excess of the barriers for single layer diffusion.

We have used the Scanning Tunneling Microscopy (STM) to characterize the real space structure of the Au(111) surface during sputter erosion, and how it depends on incident ion energy and angle. We have also used X-ray scattering and STM to study the thermal relaxation of the sputter-induced features subsequent to their formation. Relaxation is integral not only to the growth process, but to determining the stability of nano-scale features, once created.

(Note that the title and objectives have been modified slightly from the original proposal to include the studies described above under Surface Processing with Ion Beams.)

Thin Film Growth Studies:

Our second major area of research focused on understanding how surface structure evolves during thin film *deposition* with energetic ions. Since metals and magnetic multi-layers are routinely deposited using sputter techniques (which employ hyperthermal particles), films have been grown with highly controlled energetic ions in the energy range relevant to sputter deposition to assess how the energetic beams modify growth modes, surface structure, and interface structure. We have focused our efforts on the growth of Cu on Cu(111) for reasons of technological importance. We have constructed a new hyperthermal beam line that gives us a high degree of control over incident beam conditions (e.g. species, energy and angle) during film growth. (See Section 2E - Hardware Development). Many of the experimental and analysis techniques we developed for our sputtering studies (see above) have been used for these thin film growth studies as well.

We have deposited films a few layers thick, and measured the resulting surface morphology with in-situ STM. Our goal is to understand how energetic deposition influences interlayer mass transfer and the competition between smooth 2D and rough 3D growth. Thermal deposition of Cu/Cu(111), for example, proceeds in a 3D rough mode over a wide range of substrate temperatures due to relatively high energy barriers for interlayer mass transfer. Using a state-of-the-art Molecular Dynamics/Monte Carlo simulation [7] we have predicted beam-induced 3D to 2D transitions. Experiments with energetic deposition have shown a suppression of the 3D-growth mode at room temperature due to beam-induced microscopic smoothing processes [6].

3) ACCOMPLISHMENTS/NEW FINDINGS

Our accomplishments for the period 15 December 97 – 14 December 00 can be summarized in five key areas. They are:

A. Morphology evolution of ion-irradiated Au(111);
B. Thermal relaxation of a sputter-roughened surface;

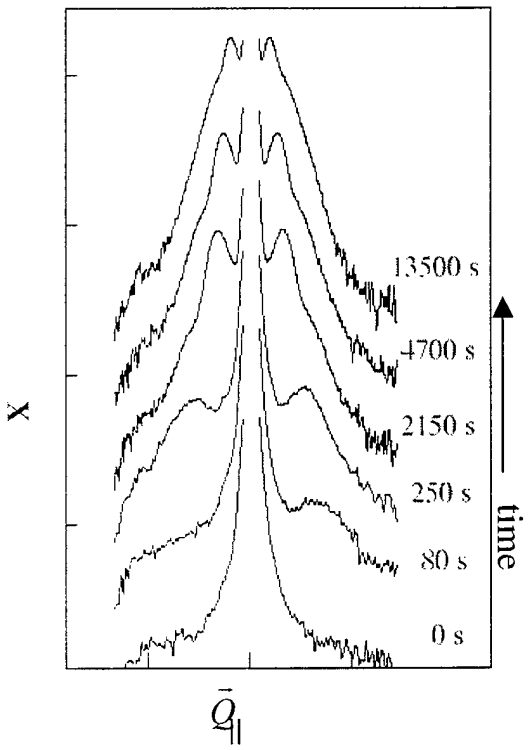


Figure 1: Low angle x-ray intensity as a function of time during ion erosion of Au(111). The ion beam eroded at a rate of .042 ML/min. and was incident at 45°. The sample temperature was 35°C.

C. Energetic deposition of Cu on Cu(111)
D. Monte Carlo and Molecular Dynamics simulations of mound formation, thermal relaxation, and energetic deposition; and
E. Hardware development for studies of energetic deposition with controlled energy beams.

(A) Morphology Evolution of Ion-Irradiated Au(111):

We have used real-time X-ray scattering and scanning tunneling microscopy (STM) to study how surface morphology evolves on the Au(111) surface during Ar^+ ion irradiation. Varying the erosion parameters (e.g., ion energy and angle, substrate temperature, and substrate species) can produce smooth, mounded, and rippled surfaces.

Significance and relevance: We have investigated how surface morphology depends on preparation conditions (e.g., ion energy and angle, substrate temperature, and substrate species). Ion sputtering is integral to technologies that involve surface cleaning, semiconductor processing, patterning, and depth profiling. We have learned what parameters produce different morphologies, to understand the microscopic mechanisms whereby energetic beams can influence morphology, and how to use ion sputtering to produce specific surface structures.

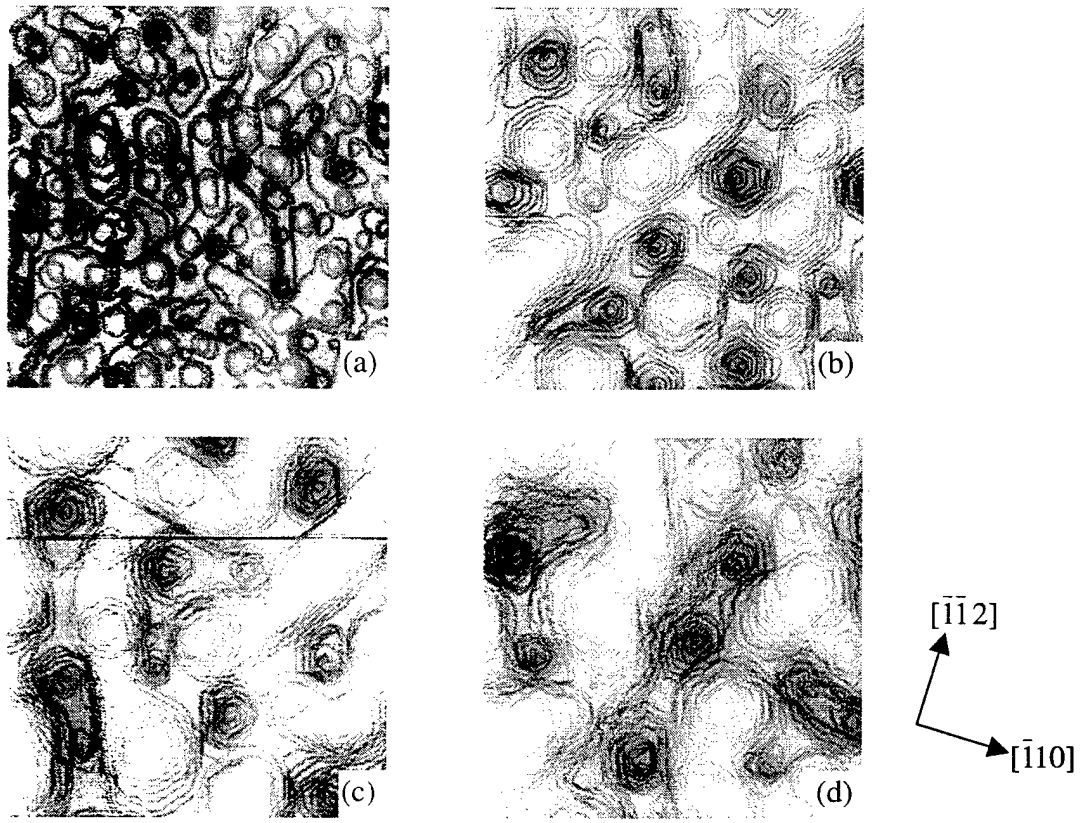


Figure 2: STM images of Au(111) eroded by 500eV Ar^+ ions. The ion flux was held constant at 3.11±. 15ML/min for all images. The sample was at 38°C during irradiation. The orientation of the crystal is shown at lower right. Number of layers removed, image size and vertical height are (a) 9.15ML, 650Å, 24Å (b) 36.6ML, 560Å, 45Å (c) 54.9ML, 650Å, 58.5Å (d) 164.7ML, 650Å, 85.5Å.

Research highlights: Key results are highlighted below.

Low temperature pattern formation: During 500 eV Ar^+ irradiation of Au(111), the morphology of the sputtered surface depends on substrate temperature. Using real-time X-ray scattering at CHESS we observe step retraction at high temperature, layer-by-layer removal at intermediate temperature, and 3D pattern formation at low temperature.

We have made the first real-time measurement of how the surface morphology evolves during low temperature sputtering. Low-angle transverse X-rays scans (see figure 1) taken during low temperature (35° C) sputtering indicate that a pattern forms on the surface with a characteristic lateral length scale. This length scale increases as a power law in time with an exponent of 0.27. This exponent is consistent with the existence of barriers for the interlayer transport of adatoms and/or vacancies that exceed the terrace diffusion barriers. The spacing ranges in magnitude from approximately 10 to 50 nm. These results are reported and discussed elsewhere [4,9]. (The X-ray work was supported jointly by this grant and by the Cornell Center for Materials Research.).

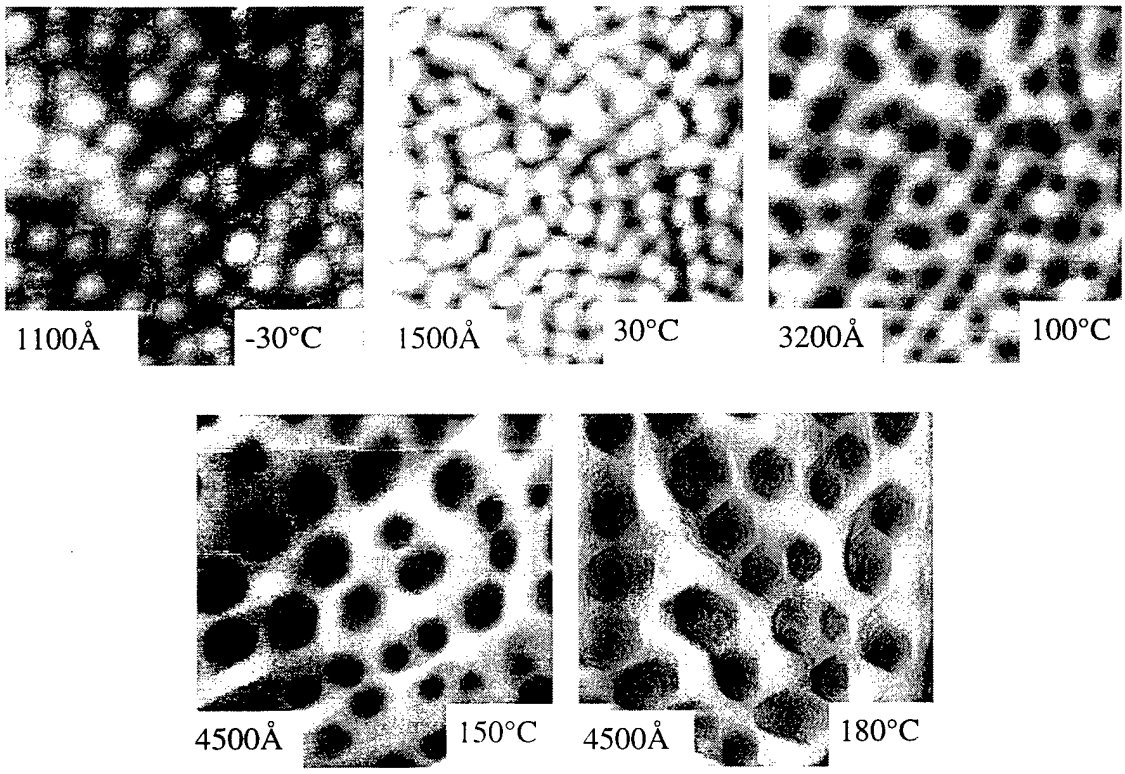


Figure 3: STM images of variable temperature ion irradiated Au(111). The sample was irradiated for 60 minutes at an erosion rate of 1.5 ML/minute, while the sample was held at a constant temperature.

While X-ray scattering is ideally suited to real-time monitoring of the average properties of the evolving surface, it does not identify real-space structures unambiguously. For example, scans such as those shown in figure 1 are unable to distinguish pits from mounds. STM, however, is ideally suited to such a task. Therefore, to complement the X-ray measurements, we have performed a series of STM measurements of surface structure evolution during Ar^+ irradiation of Au(111).

These measurements make use of an ultra high vacuum (UHV) growth (see discussion below of Hardware development in part E and figure 12). The STM can be accessed by a sample transfer system integral to the vacuum system, so that the sample can be irradiated at variable temperature and subsequently imaged while maintaining ultra high vacuum conditions.

We have performed a set of measurements of ion erosion of Au(111) at room temperature for varying lengths of time. Starting from a clean, atomically flat surface, the sample was irradiated with a constant flux of Ar ions at room temperature. Following the irradiation, the STM was used to acquire images of the sample surface (Figure 2). The auto-correlation function of the images of the sputtered surfaces was used to quantitatively obtain the average spacing between features on the surface. By obtaining a series of these images at increasing irradiation dosages, the structure of the surface features at different stages of sputtering was determined, and the characteristic spacing between the features was measured as a function of time. We have found that the length

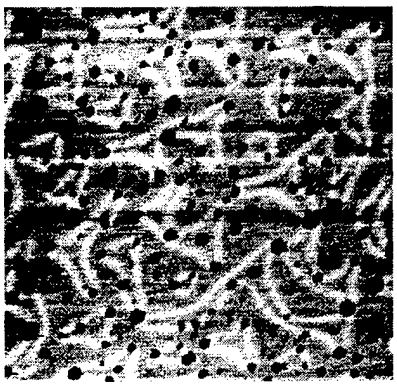


Figure 3: STM image of a single crystal Au(111) surface after the removal of 0.04 monolayers of Au with 500 eV Ar^+ sputtering. The dark holes are where material has been removed by sputtering. The light wavy lines are the remains of the surface reconstruction. Image is 640Å by 640Å.

scale of the features shown above increases with the same time dependence as observed in X-ray scattering. Because of the "stop and look" nature of the STM measurements, we expect the time evolution extracted from X-ray scattering to be more reliable. However, STM has the important advantage that the real surface structure can be characterized. This is essential for developing sophisticated patterning techniques.

We have studied the time-dependence of the ion-induced mound formation. Specific issues that we are investigating include:

Dependence of mound formation on ion flux and temperature: In addition to monitoring morphology as a function of dosage, we have investigated how the surface morphology depends on the sample temperature and on sputter ion flux. Studies were performed on Au(111) samples which were initially flat. The sample was held at a constant temperature during the erosion, and then quenched quickly to room temperature to prevent thermal annealing of the surface features. STM images of the ion-eroded surfaces were obtained for each erosion temperature (figure 3). The images demonstrate that there is a continuous change in surface morphology developed during ion irradiation from mounds at low temperature erosion to pits at high temperature erosion. We are currently using kinetic monte-carlo simulations to understand the origin of the transition in erosion morphology.

In addition, we have conducted preliminary experiments for erosion at high ion fluxes. We have found that mounds form on the surface but their separation and size no longer scale in time. (The transition occurs somewhere between removal rates of 2 and 5 monolayers/minute.)

Azimuthal ordering during mound formation: We have found that mounds formed during sputtering, similar to those shown in figure 3, often show some degree of azimuthal ordering. That is, the mounds were preferentially aligned along certain directions related to the crystallographic order of the substrate [4,9]. Under some irradiation conditions, we observe a striking degree of ordering. We have investigated the extent of ordering under

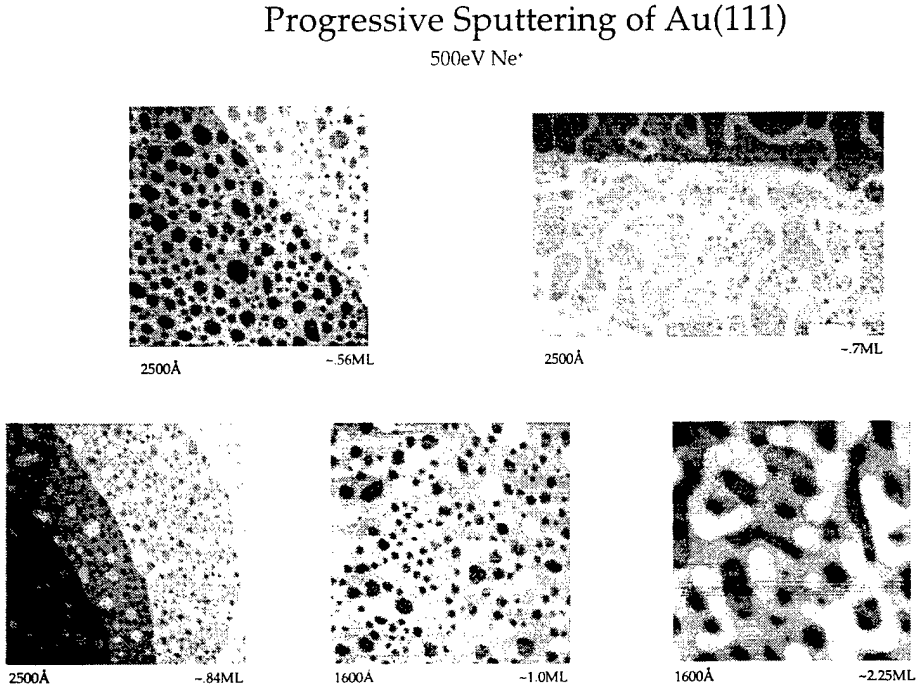


Figure 5: STM images taken after progressively increasing doses of 500 eV Ne^+ ions. Images shown are, from left to right: upper row, after 0.56 and 0.7 monolayers removed, and lower row, after 0.84, 1.0, and 2.24 monolayers removed. Different shades of gray correspond to single atomic layer height changes. with lighter being higher. Lateral dimensions of the images are given in the figure.

different experimental conditions. We have attempted to find experimental conditions in which sputtering can be used to form arrays of mounds with control over the spacing between mounds as well as their positions. Such surfaces could be used as templates for depositing ordered islands, as ways to form ordered magnetic dots, and as starting surfaces for relaxation studies.

Initial stages of mound formation: In order to develop more control over surface patterning with ion beams, it is essential to understand the early stages of the pattern formation. Our X-ray measurements indicate that, starting from an initially flat surface, the earliest measurable selected length scale during low temperature sputtering of Au(111) (see figure 1) is determined before a few monolayers have been removed. However, the time resolution we had during these X-ray scans was insufficient to provide a detailed picture of the early time development. Furthermore, the X-ray scans do not give real-space information about the surface. We have thus begun to study this early time behavior with STM.

The clean Au(111) surface exhibits the so-called herringbone reconstruction, with a long range wavelength of ~60Å. We have used the STM to monitor the earliest stages of sputter erosion on this surface. During the removal of the first 1% of the top layer, the mobility of the vacancies created by ion impacts seems to be influenced by the surface reconstruction. Following this, the vacancies begin to disrupt the reconstruction, as shown in figure 4. We are interested in confirming the observation that vacancy mobility

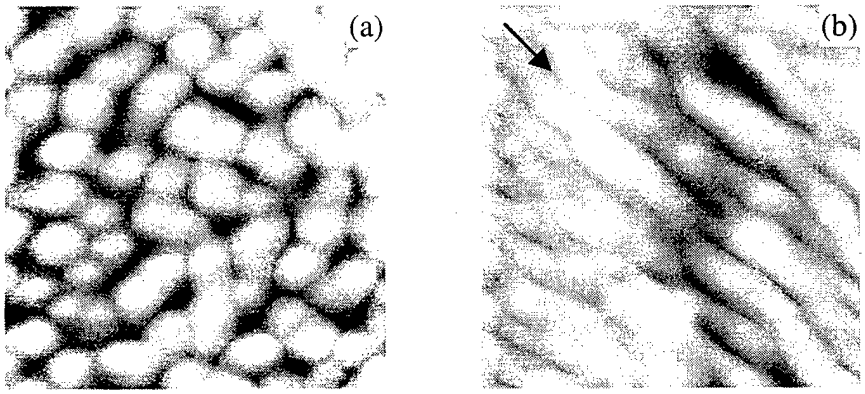


Figure 6: STM images of sequentially eroded surface. (a) Image after normal incidence erosion corresponding to 13.5 ML removed. Image size is 1000Å and lateral scale is 45Å vertical. (b) Image after 20 minutes of 15° erosion[11]. The arrow indicates the incident beam direction. The image is 1300Å lateral and 59Å vertical scale.

is affected by the surface reconstruction, as well as studying the disruption of the surface reconstruction.

As sputtering continues the appearance of the top layer changes (see figure 5). Some interesting features develop which reflect the symmetry of the underlying Au(111) surface (e.g., near a monolayer removal the step edges show evidence of structures with three- and six-fold symmetry). A correlated length scale develops in the first few monolayers of ion erosion (figure 1), even though the mounds are not yet visible (figure 5). Through analysis of the initial stages of erosion using both X-ray (figure 1) and STM (figure 5) techniques, we have investigated the mechanisms by which the initial length scale of the pattern is selected. We have also observed how the mounds, plainly evident at later states of the evolution, start to evolve, and the point at which azimuthal ordering begins to occur.

Ripple formation: During low temperature glancing angle Ar^+ erosion of the Au(111) surface, one dimensional (1D) structures develop. The 1D correlated length scale shows up in X-ray scattering as a correlation in a single azimuthal orientation. Figure 7 (left) shows glancing angle transverse X-ray scans taken during sputtering after the removal of approximately 20 monolayers. The broad diffuse scattering differs markedly for scans taken in directions parallel and perpendicular to the sputtering beam. In the parallel direction, the satellite peaks in the diffuse scattering indicate a selected length scale, whereas no such length scale appears in the perpendicular direction. Figure 7 (right) shows an STM scan of the rippled morphology, produced under conditions similar to those in Figure 7 (left).

We have investigated the origin of the ripple morphology, since ripple formation at the nm length scale occurs in many different materials. Depending on the mechanism for ripple formation, the ripples can form either parallel or perpendicular to the direction of the incoming ion beam. In X-ray and STM studies of ripple formation on Au(111), only ripples parallel to the ion beam have been observed.

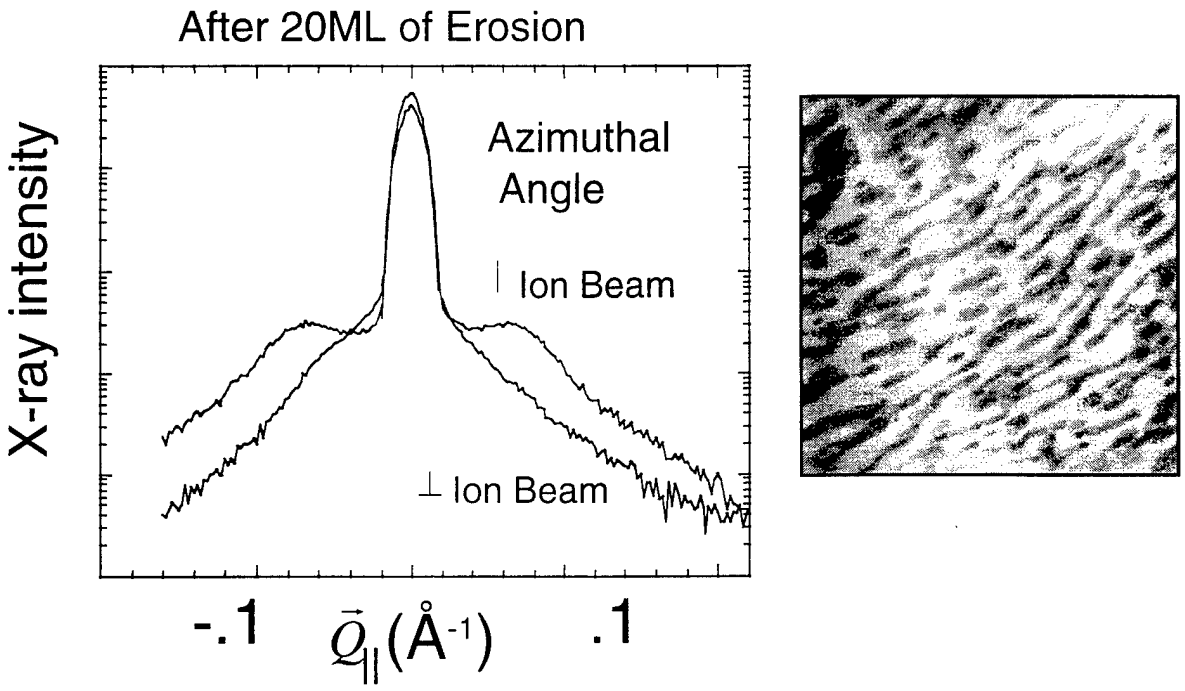


Figure 7: (Left) Low angle transverse X-ray scans taken during glancing angle (15° degrees, measured from the surface plane) 500 eV Ar^+ irradiation of Au(111) at room temperature. The X-ray intensity is shown for scans in the direction perpendicular to and parallel to the incident ion beam. The satellite peaks in the scan direction parallel to the ion beam indicate a characteristic length scale that corresponds to the spacing between ripples. **(Right)** STM image of a ripple morphology produced on the room temperature Au(111) surface by sputtering with 500eV Ar^+ ions at a glancing angle of 15° (measured from the surface plane). The image is 2500Å on a side.

We have also investigated ways to control ripple spacing and amplitude. We have demonstrated that multiple stages of erosion using a deliberate sequence of incidence angles can be used to control the final morphology. We used the average 2D length scale formed by normal incidence erosion, which can be controlled by the ion fluence, to set the average spacing of ripples on the surface. Ripples were formed during a second glancing angle irradiation. Because shadowing at glancing angles is significant, there is less erosion of the mounds aligned along the ion beam direction. The combined exposures of normal incidence and glancing angle ion bombardment were used to create ripples on the surface, as shown in figure 6. An initial dose at normal incidence sets a length scale of mounds and pits on the surface(figure 6(a)). The sample was observed with the STM before a second irradiation at 15° incidence angle. Figure 6(b) shows ripples on the surface, aligned with the orientation of the ion beam. The spacing of the ripples was approximately the same as the mound-mound spacing on the surface after normal incidence erosion, and the RMS roughness had decreased from 10.4Å to 9.9Å.

(B) Thermal relaxation of a sputter-roughened surface:

We are using X-ray scattering and STM to study the thermal relaxation of rough surfaces produced by ion sputtering.

Significance and relevance: Relaxation is the phenomenon whereby a rough surface evolves over time toward its equilibrium state. Since surfaces during growth and sputtering develop roughness, relaxation is also integral to how morphology evolves during these processes. Thermal relaxation occurs when the atom and step motions (we ignore evaporation/condensation) are thermally activated, and hence is always present. Even in energetic deposition, where morphology can be influenced by the non-equilibrium ion-surface impacts, thermal relaxation is present. Furthermore, thermal relaxation occurs subsequent to growth and/or processing and is crucial in determining the stability of any small surface features that were created.

Research highlights: Even though thermal relaxation is one of the most fundamental of surface processes, the specific mechanisms remain poorly understood. This is partly due to the difficulty of collecting high quality data that reflects surface structure over several orders of magnitude in time. We have used real-time X-ray scattering at CHESS to monitor the thermal relaxation of mounds and ripples created on Au(111) during ion sputtering. We have also used STM as a complement to the X-ray measurements in order to interpret the diffraction data.

Our goal has been to obtain high quality data that we can use to determine how the surface relaxes as a function of time. Many current theoretical models and simulations suggest that surface relaxation is a universal process describable by simple scaling laws, e.g., power laws. Furthermore, the exponents in these power laws (the scaling exponents) are determined by which microscopic processes control the relaxation. Most of these models assume that the rate-controlling processes are constant over time.

During the first year of this grant, we completed preliminary studies of the relaxation of mounds on the Au(111) surface [10]. Our goal was to monitor how the surface features relaxed over time. A sputtered surface was prepared in ultra high vacuum and subsequently monitored by a point detector, sweeping out successive low angle transverse X-ray scans at the anti-Bragg scattering condition. This preliminary work demonstrated that X-ray scattering from a high intensity synchrotron source at the anti-Bragg condition can track the surface as it relaxes. The full-width-at-half-maximum (FWHM) of the diffuse scattering at this particular scattering condition is inversely related to a lateral correlation length on the surface. It was found in our preliminary work that the FWHM decreases as the surface relaxes. However, several features of the preliminary data made it difficult to extract reliable FWHM and the time dependence of the lateral correlation length on the surface as it relaxed did not provide a definitive exponent.

To overcome several of the problems encountered in extracting reliable X-ray data using point detectors, we monitored the relaxing surface at the anti-Bragg condition using a CCD area detector. The area detector has several distinct advantages over the point detector: First, it has much better time resolution. Not only is the acquisition time less than half that of a transverse scan of the point detector, all of the diffuse scattering intensity is time averaged. In a point detector, each point of the transverse scan is actually taken at a different time, so that distortion occurs in the line-shape. Second, point detectors require slits which convolute the resulting data sets, while area detectors do not. Third, area detectors capture a larger portion of reciprocal space information.

Our sample preparation involves roughening a Au(111) surface by sputtering with 500 eV argon ions. From previous STM work, we know the erosion produces hexagonal pits and mounds with some lateral ordering. Once the sample is prepared, we monitor the approach to equilibrium continuously for 15 hours using the CCD area detector. The relaxation and erosion occur at 60º C, which we monitor with a thermocouple. We have extracted the lateral correlation length on the surface during relaxation at over 200 times during the 15 hour period and determined its time dependence: it increases with power-law behavior with an exponent of 0.23.

Coupled with our observations of the relaxing surface using STM, this exponent can not be attributed to a single feature of the surface relaxing. From STM movies of a similarly prepared surface relaxing at room temperature, we find faceting at mound tops and bottoms. However, we also see coalescence of surface features that leads to facets increasing in size, producing a coarsening of the pattern. That is mounds and pits random walk on the surface and collide (they random walk by means of fluctuations of the step edges which require very fast edge diffusion). To date, this coalescence has not been included in any thermal relaxation models.

We have used Monte Carlo modeling to study the relaxation of 1D and 2D periodic structures at temperatures below the roughening transition [11] (see Part 4 of this section.)

(C) Energetic deposition of Cu on Cu(111)

Significance and Relevance: Modern technology relies on hyperthermal ion deposition techniques in a variety of systems: sputter deposition (PVD) of copper interconnects used in mainstream computer processors, cobalt and copper for hard drive read heads, and a variety of ion milling and sample preparation techniques. While technology has employed the use of these low energy ions, understanding the mechanisms has been incomplete. These experiments and simulations provide important clues for understanding why the techniques used provide better quality films than the preceding methods.

Research Highlights: While films of silver (Ag), cobalt (Co), and copper (Cu) have been grown using our direct ion deposition system, our scientific efforts have been focused on copper thin film deposition. Films have been grown between10eV and 100eV at room temperature and analyzed for correlations with atomistic mechanisms predicted by the simulations described below.

As shown in Figure [8], dramatic morphological variations can be observed as a function of energy even in the first 100 eV. At 10 eV films resemble those grown with thermal deposition, i.e. they are well-separated objects with "wedding cake" morphology and a narrow distribution of object sizes. At 20 eV, the films are very similar, but the edge contours have begun to exhibit an increased complexity (not nice circular contours), and some very small vacancy islands can be observed. At 30 eV, vacancy islands are easy to identify, and the contours have both convex and concave line-shapes. The 40 eV films exhibit an abundance of pits or vacancy islands with similar contours as those in the

30eV images. At 60 eV, the films are qualitatively similar to 40eV, but the mean vacancy island size has increased, and the contours are often very distended. At 100 eV, the morphology maintains many of the two dimensional properties of the lower energy films, but is no longer as symmetric in the vertical direction. The mound-like objects have flat tops and occupy most of the surface area, while pinholes and crevasses occupy much less surface area, but are often twice as deep as the number of layers deposited.

We believe the images in Figure [8] can be interpreted from the simulation data in Figure [10] to form two conclusions:

(1) Below 20 eV, energetic insertion is the dominant non-equilibrium mechanism. Since this mechanism tends to smooth a system, which at low coverage is already smooth, the morphology looks very similar to thermal deposition. The molecular dynamics data in Figure [10] suggest an onset of adatom/vacancy formation between 20 and 30 eV, and significant vacancy islands appear in the experimental images in this energy range. We believe the appearance of these islands is direct evidence of the activation of the adatom/vacancy mechanism. Above 30 eV, the coarsening of vacancy islands can be attributed to the steadily increasing adatom/vacancy yield as predicted by the molecular dynamics.

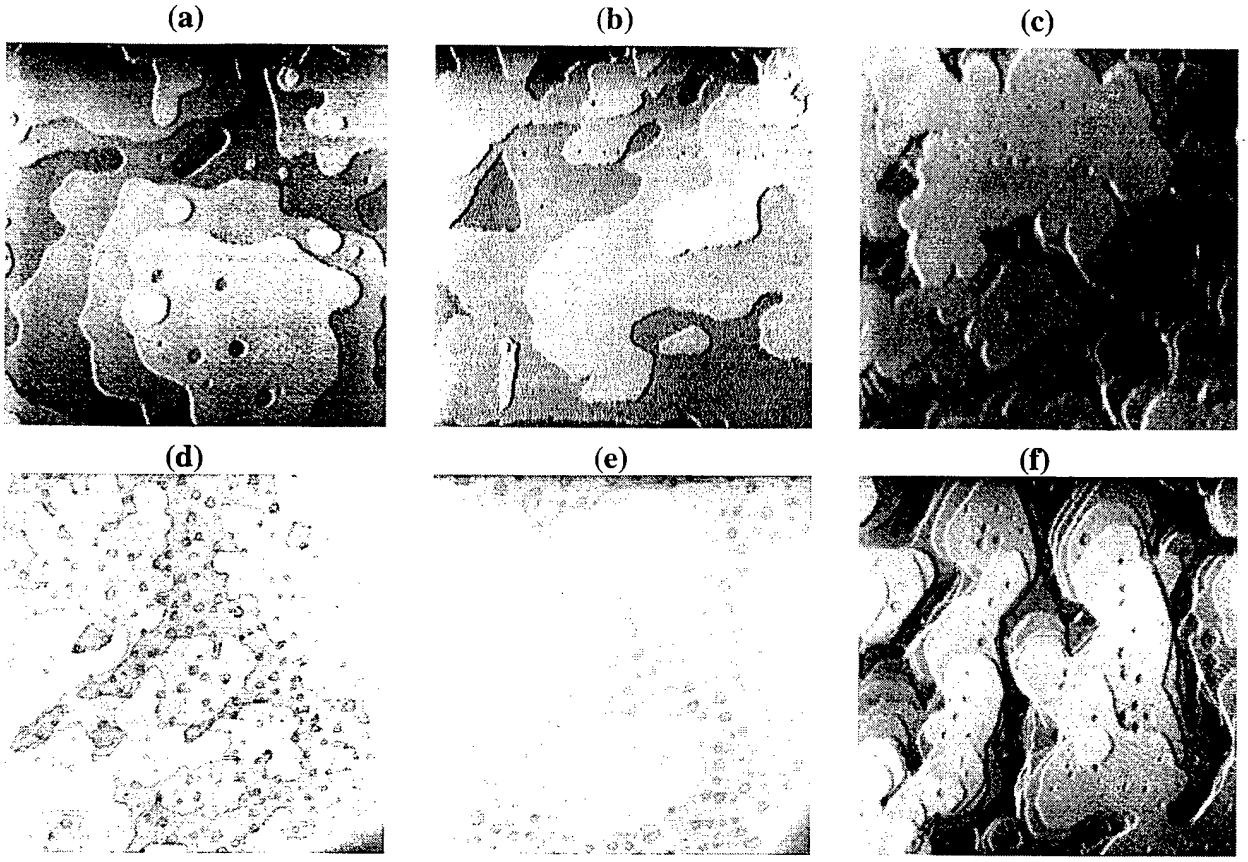


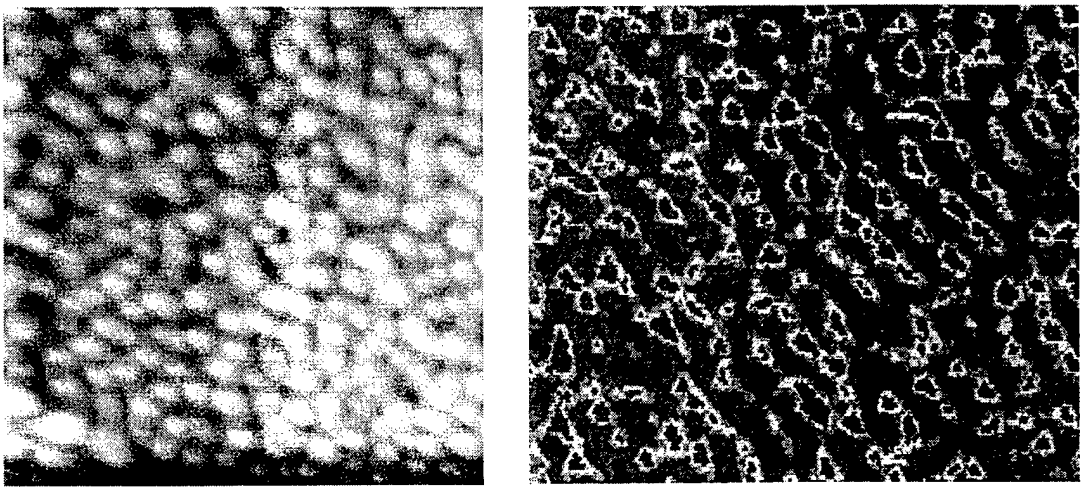
Figure 8: STM topographs of Cu(111) surfaces following ~4 monolayers of direct ion deposition at room temperature. All images are 200x200 nm and represent deposition at (a) 10 eV, (b) 20 eV, (c) 30 eV, (d) 40 eV, (e) 60 eV, and (f) 100 eV.

(2) Between 60 and 100 eV, increasing adatom/vacancy formation can no longer account for the dramatic changes in morphology. However, the molecular dynamics simulations suggest that sputter erosion becomes an important mechanism in this energy range. In addition, further analysis of molecular dynamics simulations suggests an increased probability for sputtering near step edges in this energy range. While this study is incomplete, we believe the morphological changes in this energy regime are due to the onset of sputter erosion. Further, we speculate that a preference for sputtering at step edges would lead to a morphology which has the up-down asymmetry exhibited in our films deposited at 100 eV.

(D) Monte Carlo and Molecular Dynamics simulations of energetic growth and pattern formation:

Simulations have played an important role in all of the studies discussed above.

Significance and relevance: The ability to combine highly sophisticated simulations of energetic deposition and processing with experiments using controlled beams provides a powerful means of studying the effects of energetic beams on growth modes and surface properties. We have used the simulations to identify regimes of optimal parameters for



(a) (b)

Figure 9: Image (a) is an STM topograph of a Au(111) surface after many mono-layer of 500 eV Ar^+ ion erosion. Figure (b) is an artificial image generated from the Kinetic Monte Carlo sputter erosion simulation. Many of the qualitative features of the images are the same, e.g. the relative size of the objects compared to the spacing, and the overall angular orientation.

growth, and to guide experimental efforts. The simulations have become predictive tools for film growth and surface structure optimization.

Research highlights: We use simulations in four ways.

Monte Carlo simulations of the microscopic origins of morphology evolution: Using a Monte Carlo simulation and idealized tables of energy barriers for different atomic moves, we have simulated morphology evolution under a variety of conditions relevant to our experimental program. We have investigated thermal relaxation of surfaces patterned in one and two dimensions [11], the relative roles of mobile vacancies and adatoms in determining surface structure during sputtering [12], and mechanisms of pattern formation [13]. The goal of these studies is to identify key microscopic mechanisms that control morphology evolution. For example, in recent simulations we have found that mound formation can occur when the energy barriers for atoms to diffuse off the corners of step edges are larger than those for diffusion along the step edge. Such enhanced corner barriers give rise to diffusion bias currents for adatom motion during deposition, and vacancy motion during sputtering, and can result in mound formation on the surface.

Kinetic Monte Carlo simulations of sputter erosion: Using the idealized table of energy barriers for different atomic moves and introducing symmetry breaking non-equilibrium phenomena (sputtering source) we have been able to monitor steady-state surface configurations. The simulation allows the user to adjust the number of vacancies, adatom/vacancy pairs, and range of occurrence per incident energetic particle and evolve the system between collisional events with surface kinetics appropriate to the system temperature. Existing literature [16] provides initial guidance for choosing these parameters in a physical regime, and resulting simulation surfaces closely resemble experimentally observed systems (see Figure 9.)

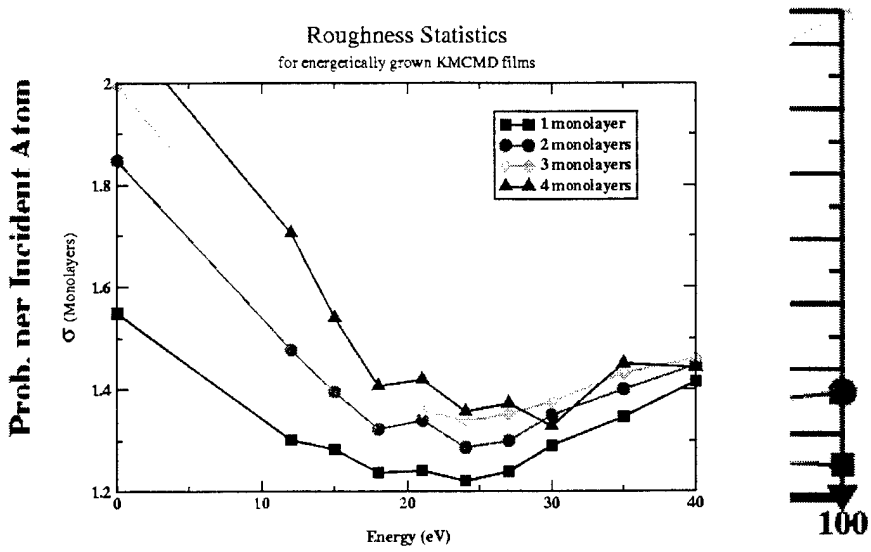


Figure 11: Several copper films were grown at 80°K on a Cu(111) crystal in the Kinetic Monte Carlo/Molecular Dynamics hybrid simulation described in Section 2D. RMS roughness measured from those films indicates an optimal energy window for growing thin films between 20-30 eV.

Molecular Dynamics Simulations of Collisional Dynamics during energetic collisions: Using Effective Medium Potentials and Molecular Dynamics routines available [17], we have developed a novel technique for developing statistics of hyperthermal collisions. The initial system consists of a "bowl" of atoms which has a (111) surface and bottom face, with six side facets tapering to the bottom. This bowl has fully active dynamics which is surrounded by a bowl with static atoms to mimic the bulk lattice. An intermediate region of critically damped Langevin atoms is placed between the dynamic and static atoms resulting in a structure which provides almost no energetic reflections and accurately models a bulk crystal. A single step edge is placed on the surface and an atom with the kinetic energy of interest is propelled toward the surface. In order to develop comprehensive statistics of a typical surface, an atom is propelled at a random position within a single unit cell of the surface for a hundred or more times. The selected position of this unit cell is then translated from well above, across, and finally below the step edge. Averaging over the statistics for all of the individual positions at every energy provides a way to identify the activation of specific events as a function of energy as shown in Figure 10. In particular, we believe the kinetic smoothing of atomic insertion is dominant below 20 eV, where energetic adatom/vacancy pair formation becomes important. The adatom/vacancy yield increases steadily above 20eV, and above 50 eV the yield for re-sputtered atoms begins to become important as well.

Molecular Dynamics/Kinetic Monte Carlo simulations of energetic beam deposition: We have developed a state-of-the-art code for simulating film growth with energetic ions [7]. The several pico-second period following each energetic ion collision with the surface is treated realistically using Molecular Dynamics (as described in the previous section), whereas the thermally activated motions of the surface atoms, with time scales up to seconds, are handled with Kinetic Monte Carlo. The two main advantages of this

hybrid technique are that: 1) the non-equilibrium atomic motions resulting from the collisions are handled by a Molecular Dynamics code, and thus result from simulations using realistic forces between surface atoms, and not from a generic table of atomic motions; and 2) time scales from sub-pico-seconds (during the collision of the incident particle) to tens of seconds (to deposit a monolayer) can be handled in a single simulation. Using this code we have identified mechanisms whereby energetic deposition can be used to promote flat 2D growth in a system where thermal deposition would result in rough 3D growth. In particular, we have identified a re-entrant layer-by-layer regime at low temperatures in fcc metals activated by energetic particles in the 20-25 eV range as shown in Figure 11. This information has guided our initial choice of experimental parameters in our studies of the deposition of ultra-thin metal films with mass- and energy-selected metal ion beams (see Section 2C above).

(The described simulations were developed with funding from the Cornell Center for Materials Research).

(E) Development/hardware for energetic deposition with controlled energy beams:

In the following we describe hardware development that has occurred in this reporting period.

Significance and relevance: In most commercial applications of energetic deposition techniques (e.g., sputter and plasma deposition), particles with a broad range of species and energies impinge on the growth surface. We are developing new sources, and experimental chambers to accompany them, that will allow us to use beams with a high degree of control of the deposition or processing parameters. For example, our new hyperthermal beam line (see discussion below and figure 12) is one of a small number of such instruments world wide that controls hyperthermal energy beams to be deposited on growth substrates in ultra high vacuum.

Research highlights: Several aspects of our experimental facilities are described below.

Growth chamber with in-situ STM: The STM images presented above were taken in our ultra high vacuum system (see figure 12), which operates in the mid 10^{-11} Torr pressure range. The system is configured so that we can prepare substrates, ion-irradiate them or deposit thin films on them, and subsequently image them within the same vacuum system. The STM is a commercial (Omicron) microscope capable of storing multiple tips and samples in vacuum. The STM system may be vacuum isolated from the deposition analysis chambers (see figure 12), allowing for the use of feed and deposition gases while keeping the STM clean.

The transfer system is designed to move the sample rapidly between the STM and the analysis and deposition chambers, where thin film growth, ion irradiation, and sample characterization are performed. The manipulator in the deposition chamber has the ability to control the temperature of the sample from -150°C to 1100°C. The analysis chamber includes an Auger spectrometer to monitor the surface composition. The system is also equipped with a residual gas analyzer and ion gauges.

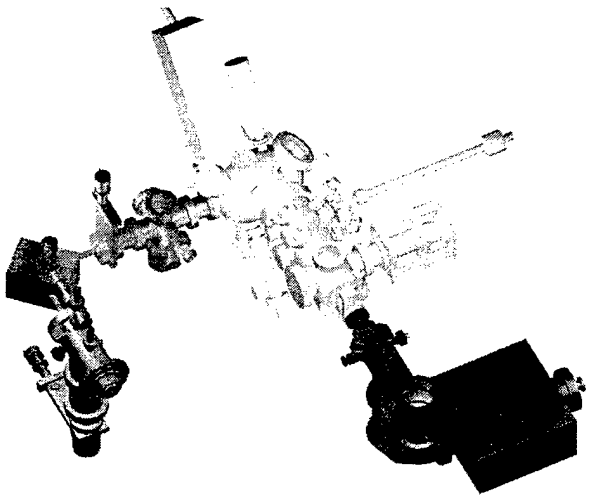


Figure 12: New ultra high vacuum/STM growth and processing system. Color coding corresponds to: violet—STM, sample and tip storage, and ion pump with isolation valve; lime—analysis chamber with Auger, residual gas analysis, thermal evaporators, deposition chamber, thin –film deposition stage including temperature control; red – mass- and energy-selected ion beam for film deposition. Samples are transferred between chambers using a sample transfer arm.

STM electronics, image collection and manipulation: The UHV-STM system operates using electronics and software constructed in-house. During image collection the STM uses an analog feedback loop to maintain the tunneling current, while the scanning signals and data collection is controlled by software. Image analysis can be performed immediately: on-line image analysis includes standard operations such as background subtraction and lighting of images, as well as more complex manipulations, such as Fourier analysis of images. On-line Fourier analysis is important in our studies of scaling during mound formation so that we can immediately determine the quality of the STM images by calculating the corresponding auto-correlation functions.

Tip preparation and cleaning station: The quality of the STM tips used to image mounds formed on sputtered surfaces is particularly important. The STM tip must have a high aspect ratio as well as a small radius of curvature to obtain accurate images. Dull tips can lead to image artifacts such as false bumps, shadows, and noise. A tip sharpening station was constructed to sharpen tungsten tips once they are inserted in the vacuum system.

Reflection High Energy Electron Diffraction (RHEED) System: A RHEED system has been added to the growth chamber, providing a real-time diffraction technique so that STM images can be correlated with different macroscopic stages (e.g., during layer-by-layer deposition) of film deposition. This system is interfaced with a computer to allow real time full image acquisition with a high-resolution digital camera system.

Thermal evaporation stage: An evaporation stage has been built for thermal depositions at temperatures up to 1500°C and with temperature control with less than one degree Celsius deviation. A shutter system allows for precise start/stop control, and allows for out-gassing and stabilization of the evaporator without sample contamination.

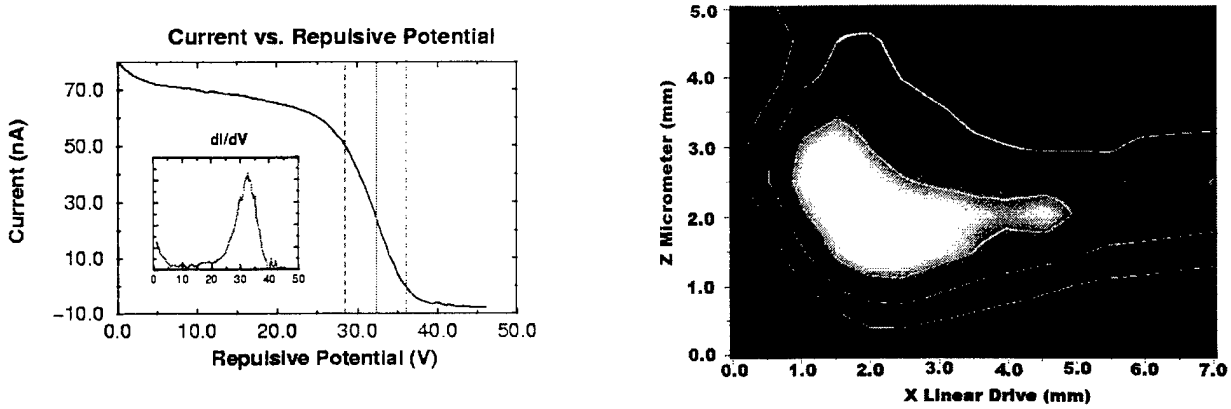


Figure 13: (Left) Ion current as a function of repulsive potential applied to the collector. The derivative of this function (inset left) is the distribution of ion energies, approximately 5 eV FWHM at 30 eV. **(Right)** Scanning a small aperture and linearly interpolating the acquired data created this spatial map of the ion beam.

Mass- and energy-selected ion beams for thin film deposition: We have completed construction of a new hyperthermal energy ion beam for thin film deposition studies. The beam line is capable of producing beams of noble gas, metal, semiconductor, and reactive ions with energies ranging from less than 10 eV to the keV range. The final beams are energy-and mass-selected, giving a high degree of control over growth parameters. Our studies have used metal ion beams. The metal ions are generated in a Penning ionization source (PIG source) by sputtering a cathode made from the desired metal with noble gas ions inside the source. Both the metal and noble gas ions are extracted. Mass selection is achieved with a double-focusing homogeneous magnetic sector field. The source and magnet were custom-built for us by Physicon Corporation. The beam line and deceleration optics (designed and built in-house) are differentially pumped with a turbo-molecular pumps so that ultra high vacuum is maintained at the sample position during deposition.

We have successfully grown Cu, Co, and Ag films on Si(100) substrates with ion energies in the range of a few eV to 40 eV. Rutherford Back-scattering Spectroscopy was used to check the deposition rates and to verify that the deposited beams showed no evidence of contamination either from vacuum contaminants (such as carbon or neon) or from beam line contaminants (such as Fe from the chamber walls or Cu from previous depositions). The energy resolution of the beam has been measured to be 5 eV FWHM at 30eV with a 200 nA current and a ~1 mm^2 spatial distribution (see Figure 13). The beam line is installed on the growth system, as shown in figure 12.

New hyperthermal ion source for thin film deposition: A new compact hyperthermal metal ion source for film growth studies has been partially constructed. It is based on source designs previously reported in the literature [14,15]. The source uses a thermal deposition furnace to generate a high flux of neutrals, some of which are subsequently ionized by magnetically confined electrons from a hot filament. The ions are extracted through a small aperture and the energy is controlled by a tunable extraction voltage. The extracted ions are collimated for transport and focussed onto the sample. Deposition can be computer controlled (see below). The advantage of this source over the one

described above (see figure 12) is its small size, which will be highly advantageous for our real-time growth studies at the CHESS, where space limitations are severe.

Computer control of the growth system: A PC-based computer system has been developed for automated data collection and analysis, including image processing, system control, and feedback. The PC's key role has been raw data collection and analysis with the RHEED system. The PC will allow long time and real-time analysis of RHEED spot diffraction intensities, providing key information for coordinating the STM data with different stages of film growth. The PC is also used to automate collection of routine system data, Auger data for quantitative comparison of different scans, and for Residual Gas Analysis data collection. Beam characterization of quantities such as spatial profiles, energy distribution, and current monitoring and feedback during deposition are also done via the PC's data collection suite.

3) PERSONNEL SUPPORTED

Graduate students supported by this grant:

Tatjana Curcic – supported Spring and Summer 1997
Aaron Judy -- supported Summer (partial) and Fall 1997, Spring, Summer, and Fall 1998, Spring, Summer (partial), and Fall 1999.
Evelyn Butler -- supported Summer (partial) and Fall 1997; Spring and Summer(partial) 1998; Summer (partial) and Fall 1999.
Chad Sosolik -- supported Fall 1999 (partial).

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Arthur Woll (supported by the Cornell Center for Materials Research)
Josh Pomeroy (supported by the Cornell Center for Materials Research)
Colin Hill (supported by the Cornell Center for Materials Research)

Post-Docs associated with the research effort:

Dr. M.V. Ramana Murty (supported by the Cornell Center for Materials Research)
Dr. Joachim Jacobsen (supported by the Cornell Center for Materials Research)
Dr. Oana Malis (supported by the Cornell Center for Materials Research)
Dr. Markus Rauscher (supported by the Cornell Center for Materials Research)

Faculty associated with the research effort:

Dr. James P. Sethna, Department of Physics

Dr. Joel D. Brock, School of Engineering & Applied Physics
Dr. Jack Blakely, Department of Materials Science & Engineering

Senior collaborators associated with the research effort:

Dr. Randy Headrick (staff scientist, Cornell High Energy Synchrotron Source)
Dr. Stefan Kycia (staff scientist, Cornell High Energy Synchrotron Source)
Dr. Kit Umbach (senior research associate, Department of Materials Science & Engineering)

4) PUBLICATIONS

J.G. McLean, B. Krishnamachari, D.R. Peale, E. Chason, J.P. Sethna, and B.H. Cooper, *Decay of Isolated Surface Features Driven by the Gibbs-Thomson Effect in an Analytic Model and A Simulation*, Phys. Rev. B **55**, 1811 (1997).

D.M. Goodstein, E.B. Dahl, C.A. DiRubio, and B.H. Cooper, *Trapping of Ions at Metal Surfaces*, Phys. Rev. Lett. **78**, 3213 (1997).

E.B. Dahl, D.M. Goodstein, C.A. DiRubio, and B.H. Cooper, *Trapping at Hyperthermal Energies*, Nucl. Instrum. and Meth. Phys. Res. B **125**, 237 (1997).

J.G. McLean, B. Krishnamachari, E. Chason, D.R. Peale, J.P. Sethna, and B.H. Cooper, *A Model and Simulation of the Decay of Isolated Nanoscale Surface Features*, (in Surface Diffusion: Atomistic and Collective Processes, ed. M.C. Tringides, NATO-ASI proceedings, Plenum Press, New York, 1997), pp. 377-388.

E.B. Dahl, E.R. Behringer, D.R. Andersson, and B.H. Cooper, *The Connection Between Multi-State Resonant Charge Transfer Dynamics and Many-Electron States in Atom-Metal Scattering*, Intl. J. Mass. Spec. Ion Proc. **174**, 267 (1998).

M.V. Ramana Murty, T. Curcic, A. Judy, B.H. Cooper, A.R. Woll, J.D. Brock, S. Kycia, and R.L. Headrick, *X-Ray Scattering Study of the Surface Morphology of Au(111) During Ar^+ Ion Irradiation*, Phys. Rev. Lett. **80**, 4713 (1998).

C.A. Keller, A.C. Lavery, and B.H. Cooper, *Positive and Negative Ion Formation in Low Energy O^+ - Cu(001) Scattering*, Phys. Rev. B, **58** 10959 (1998).

M.V. Ramana Murty and B.H. Cooper, *Surface smoothing during sputtering: mobile vacancies versus adatom detachment and diffusion*, Surf. Sci., **415** 328 (1998).

Joachim Jacobsen, B.H. Cooper, and James P. Sethna, *Simulations of energetic beam deposition: From picoseconds to seconds*, Phys. Rev. B,**58** 15847 (1998).

M.V. Ramana Murty, T. Curcic, A. Judy, B.H. Cooper, A.R. Woll, J.D. Brock, S. Kycia, and R.L. Headrick, *Real-Time X-Ray Scattering Study of Surface Dynamics on*

Au(111) During Ar^+ Ion Irradiation, Mechanisms and Principles of Epitaxial Growth in Metallic Systems, 195 (1998).

A.C. Lavery, C.E. Sosolik, C.A. Keller, B.H. Cooper, *Charge Transfer Dynamics of Low Energy Oxygen Ion Beams Scattered from Cu(001)*, Nucl. Instrum. Meth. B **157** 42 (1999).

A.C. Lavery, C.E. Sosolik, B.H. Cooper, *Energy- and Angle-Dependent Trends in the Trapping Probability of O^+ Incident on Cu(001),* Nucl. Intrum. Meth. B **157** 214 (1999).

M.V. Ramana Murty and B.H. Cooper, *Instability in molecular beam epitaxy due to fast edge diffusion and corner diffusion barriers*, Phys. Rev. Letters **83** 352 (1999).

A.C. Lavery, C.E. Sosolik, B.H. Cooper, *Energy- and Angle-Dependent Trends in the Trapping Probability of O^+ Incident on Cu(001),* Nucl. Intrum. Meth. B 157 214 (1999).

A.Judy, M.V. Ramana Murty; E. Butler; B.H. Cooper; A.R. Woll; J.D. Brock; S. Kycia; R.L. Headrick, *Real-time X-ray scattering study of surface morphology evolution during ion erosion and epitaxial growth of Au(111),* Phys. Rev. B, **60** 16956 (1999).

A.C. Lavery, C.E. Sosolik, B.H. Cooper, *Corrugation Effects in Oxygen Surface Trapping at Hyperthermal Energies,* Phys. Rev. Lett. **83** 5286 (1999).

A. Judy, M.V. Ramana Murty; E.N. Butler; J.M. Pomeroy, B.H. Cooper; A.R. Woll; J.D. Brock; S. Kycia; R.L. Headrick, *R oughening of Au(111) surfaces during ion beam erosion: a scanning tunneling microscope and X-ray diffraction study,* Epitaxial Growth-Principles and Applications, 61 (1999).

A.C. Lavery, C.E. Sosolik, C.A. Keller, B.H. Cooper, *Charge Transfer and Memory Loss in keV Oxygen-Ion Scattering from Cu(001)*, Phys. Rev. B **61** 2291 (2000).

M.V. Ramana Murty; A.J. Couture; B.H. Cooper; A.R. Woll; J.D. Brock; R.L. Headrick, *Persistent layer-by-layer sputtering of Au(111),* J. Appl. Phys., **88** 597 (2000).

C.E. Sosolik, A.C. Lavery, E.B. Dahl, B.H. Cooper, *A Technique for Accurate Measurement of Ion Beam Current Density Using a Faraday Cup,* Rev. Sci. Instrum. **71** 3326 (2000).

A.C. Lavery, C.E. Sosolik, B.H. Cooper, *Surface Trapping During Hyperthermal Energy Scattering*, Phys. Rev. B, **62**, 16126 (2000).

J.M. Pomeroy, A. Couture, J. Jacobsen, C.C. Hill, J.P. Sethna, B.H. Cooper, and J.D. Brock, *STM characterization of Cu thin films grown by direct ion deposition,* Proceeding of the Materials Research Society Session P, Fall 2000, in press.

C.E. Sosolik, B.H. Cooper, *Heavy Atom-Surface Scattering at Hyperthermal Energies,* accepted for publication in Nucl. Instrum. Meth. B.

A.J. Couture, E.N. Butler, M.V.R. Murty, J.M. Pomeroy, J.P. Sethna, B.H. Cooper, *Morphology transition during variable temperature ion erosion of Au(111),* in preparation.

A.J. Couture, E.N. Butler, M.V.R. Murty, J.M. Pomeroy, J.P. Sethna, B.H. Cooper, *The effect of Ar implantation on surface morphology of ion eroded Au(111),* in preparation.

C.E. Sosolik, J.R. Hampton, A.C. Lavery, B.H. Cooper, J.B. Marston, "Temperature Dependent Neutralization in Hyperthermal Energy Alkali-Ion Scattering from Cu(001)," in preparation.

Theses:

T. Curcic – *"Thermal Smoothing of a Rough Au(111) Surface: An X-Ray Study,"* Cornell Ph.D. Thesis (1998).

E.B. Dahl – *"Multi-State Charge transfer Dynamics and Trapping of Hyperthermal and Low Energy Alkali Ions,"* Cornell Ph.D. Thesis (1998).

A.C. Lavery – *"Charge transfer and trapping during low and hyperthermal energy oxygen ion scattering,"* Cornell Ph.D. Thesis (1999).

A.J. Couture – *"Surface morphology evolution during ion erosion of metal surfaces: scanning tunneling microscope studies,"* Cornell PhD Thesis (2000).

5) INTERACTIONS/TRANSITIONS

a) **Participation /presentations at meetings, conferences, seminars, etc.**

Contributed talk at the March Meeting of the American Physical Society, Kansas City, MO, March 1997, "Evolution of Surface Morphology During Ion Irradiation" (presented by M.V. Ramana Murty).

Contributed talk at the March Meeting of the American Physical Society, Kansas City, MO, March 1997, "New Method for Stimulating Growth by Energetic Deposition" (presented by J. Jacobsen).

Contributed talk at the March Meeting of the American Physical Society, Kansas City, MO, March 1997, "Charge transfer Dynamics of Low Energy Reactive Ion Beams Scattered from Cu(001)" (presented by A.C. Lavery).

Contributed talk at the March Meeting of the American Physical Society, Kansas City, MO, March 1997, "Excited State Formation in Atom-Surface Scattering" (presented by C. Sosolik).

Physics Department Colloquium, University of Delaware, March 1997, "Atom-Surface Interactions: Probing Dynamics with Scattering" (presented by B.H. Cooper).

Physical Electronics Conference, Eugene OR, June 1997, "X-Ray Studies of Sputtering and Growth of Au(111)," (presented by M.V. Ramana Murty).

University of Houston Seminar, Houston, TX, "Excited State in Li^+ Scattering and Preliminary Results from keV Oxygen Ion Scattering Experiments," (presented by C.E. Sosolik.)

Gordon Conference on Materials Processing Far From Equilibrium (Invited Talk), Meriden, NH, August 1997, "Surface Evolution Induced by Ion Irradiation: Fundamentals and Applications to Growth and Processing" (presented by B.H. Cooper).

Gordon Conference on Dynamics at Surfaces, Andover, NH, September 1997, Participant and poster presentation (presented by B.H. Cooper).

Workshop on Atomic, Molecular, and Optical Physics, Chantilly, VA, September 1997, Invited Participant (B.H. Cooper).

Industrial Review and Worksop, University of Maryland MRSEC, College Park, MD, September 1997, Invited Participant (B.H. Cooper).

Materials Research Society, Fall Meeting, Boston, MA, December 1997, "Surface Dynamics During Sputtering," (presented by M.V. Ramana Murty).

Contributed talk at the March Meeting of the American Physical Society, Los Angeles, CA, March 1998, "Surface Dynamics on Au(111) During Ion Bombardment," (presented by M.V. Ramana Murty).

Contributed talk at the March Meeting of the American Physical Society, Los Angeles, CA, March 1998, "Sputter Erosion of Au(111): X-ray Studies and Scanning Tunneling Microscopy (STM)," (presented by A. Judy).

Contributed talk at the March Meeting of the American Physical Society, Los Angeles, CA, March 1998, "Oxygen Trapping at a Cu(001) Surface," (presented by A.C. Lavery).

Contributed talk at the March Meeting of the American Physical Society, Los Angeles, CA, March 1998, "Charge Transfer Dynamics of Low Energy Oxygen Ion Beams Scattered from Cu(001)," (presented by C. Sosolik).

Presentation to the membership of the Cornell Center for Materials Research, Cornell University, April 1998, "Extended nm-Scale Surface Pattern Evolution" (presented by B.H. Cooper).

Materials Research Society, Spring Meeting, San Francisco, CA, April 1998, "Dynamics on the Au(111) Surface During Ion Bombardment," (presented by M.V. Ramana Murty).

Cornell University Department of Physics Seminar, Ithaca, NY, June 1998, "Trapping Trends in Hyperthermal Energy Oxygen Scattering from Cu(001)," (presented by A.C. Lavery.)

Physical Electronics Conference, State College, PA, June 1998, "Pattern Formation During Ion Irradiation and Molecular Beam Epitaxy," (presented by M.V. Ramana Murty).

Cornell High Energy Synchrotron Source (CHESS) Users Workshop, Ithaca, NY, June 1998, "Sputter Erosion of Au(111): X-Ray Studies and Scanning Tunneling Microscopy," (presented by A. Judy).

Cornell High Energy Synchrotron Source (CHESS) Users Workshop, Ithaca, NY, June 1998, "Pattern Formation during Ion Irradiation of Au(111)," (presented by M.V. Ramana Murty).

Cornell High Energy Synchrotron Source (CHESS) Users Workshop, Ithaca, NY, June 1998, "Nanometer-Scale Sputter-Induced Rippling of the SiO_2 Surface Characterized with Real-Time X-Ray Scattering," (presented by K. Umbach).

Argonne National Laboratory, Materials Division, Argonne, IL, August 1998, "Pattern Formation During Sputter Erosion and Molecular Beam Epitaxy," (presented by M.V. Ramana Murty).

Materials Research Society, Fall Meeting, November1998, "Sputter Erosion of Au(111), X-ray and STM studies," (presented by Aaron Couture.)

Materials Research Society, Fall Meeting, November1998, "Energy Dependent Trapping Probabilities of Hyperthermal O^+ on Cu(001)," (presented by C.E. Sosolik.)

International Workshop on Inelastic Ion-Surface Collisions, South Padre Island, Texas, January 1999, "Oxygen Trapping at the Cu(001) Surface," (presented by A.C. Lavery.)

International Workshop on Inelastic Ion-Surface Collisions, South Padre Island, Texas, January 1999, "Charge Transfer Dynamics of Low-Energy Oxygen Ion Beams Scattered from Cu(001)," (presented by C.E. Sosolik.)

Cornell University Chemistry Department Seminar, Ithaca, NY, February 1999, "Collisional Dynamics of Oxygen and Carbon Ions Scattered from a Cu(001) Surface," (presented by A.C. Lavery.)

Contributed talk at the March Meeting of the American Physical Society, Atlanta, GA, March 1999, "Morphology Evolution on Au(111), STM Studies of Mound Formation," (presented by Aaron Couture).

Contributed talk at the March Meeting of the American Physical Society, Atlanta, GA, March 1999, "X-Ray Scattering and Morphology Evolution of Patterned Surfaces During Thermal Relaxation," (presented by E.N. Butler.)

Contributed talk at the March Meeting of the American Physical Society, Atlanta, GA, March 1999, "Trapping and the interaction potential in O^+ scattering from Cu(001)," (presented by A.C. Lavery)

Contributed talk at the March Meeting of the American Physical Society, Atlanta, GA, March 1999, "RHEED comparison of ultrathin Cu films grown with hyperthermal ions and thermal deposition," (presented by J.M. Pomeroy)

Contributed talk at the March Meeting of the American Physical Society, Atlanta, GA, March 1999, "Temperature Dependent K^+ and Ca^+ Scattering from Cu(001)," (presented by C.E. Sosolik.)

Materials Research Society, Spring Meeting, San Francisco, CA, April 1999, "Sputter Erosion of Au(111): X-ray Studies & Scanning Tunneling Microscopy (STM)," (presented by Aaron Couture.)

Cornell University Department of Physics Summer Seminar, Cornell University, Ithaca, NY, June 1999, "Making Mountains on Gold: Ion Erosion and Atomic Scale Roughening," (presented by Aaron Couture.)

Cornell High Energy Synchrotron Source (CHESS) Users Workshop, Ithaca, NY, June 1999, "X-ray and STM studies of ion erosion of Au(111)," (presented by Aaron Couture.)

European Science Foundation Conference – *Particle-Solid Interactions: Dynamic Phenomena*, San Sebastian, Spain, September 1999, "The Dynamics of Multi-state Charge Transfer," (presented by C.E. Sosolik.)

European Science Foundation Conference – *Particle-Solid Interactions: Dynamic Phenomena*, San Sebastian, Spain, September 1999, "Temperature Dependent Alkali Scattering Ion Scattering from Cu(001)," (presented by J.R. Hampton.)

Materials Research Society, Fall Meeting, Boston, MA, November 1999, "Thermal Relaxation of Ion Eroded Au(111) Monitored by X-Ray Scattering," (presented by E.N. Butler.)

Materials Research Society, Fall Meeting, Boston, MA, November 1999, "Variable Temperature Ion erosion of Au(111)," (presented by Aaron Couture.)

Materials Research Society, Fall Meeting, Boston, MA, November 1999, "Surface Morphology Evolution During Ion Irradiation and Annealing," (presented by M.V. Ramana Murty.)

Materials Research Society, Fall Meeting, Boston, MA, November 1999, "Surface Roughness Measurements of Films Grown Using Hyperthermal Cu^+ on Cu(111)," (presented by Josh Pomeroy.)

Contributed talk to the American Physical Society March Meeting, Minneapolis, MN, March 2000, "Temperature Dependent Neutralization in Akali and Alkaline Earth Ion-Surface Scattering," (presented by C.E. Sosolik.)

Contributed talk to the American Physical Society March Meeting, Minneapolis, MN, March 2000, "Temperature-Dependent Scattering Dynamics of Hyperthermal-Energy K^+ Incident on Cu(001)," (presented by J.R. Hampton.)

Contributed talk at the March Meeting of the American Physical Society, Minneapolis, MN, March 2000, "Deposition of Metal Thin Films Using Hyperthermal Ions," (presented by J.M. Pomeroy)

State University of New York (SUNY) at Geneseo Seminar, Geneseo, NY, 2000, "Making Mountains on Gold: Ion Erosion and Atomic Scale Roughening," (presented by Aaron Couture.)

Materials Research Society, Fall Meeting, Boston, MA, November 2000, "STM Characterization of Cu Thin Films Grown by Direct Ion Deposition," (presented by Josh Pomeroy.)

Cornell University, Department of Physics Seminar, Ithaca, NY, June 2000, "The Search for the Flying Kondo Effect," (presented by C.E. Sosolik.)

International Workshop on Inelastic Ion-Surface Collisions, San Carlos de Bariloche, Argentina, November 2000, "Heavy Atom-Surface Scattering at Hyperthermal Energies," (presented by C.E. Sosolik.)

Princeton University Department of Physics Condensed Matter Seminar, Princeton, NJ, January 2001, "Heavy Atom-Surface Scattering and the Search for the 'Flying' Kondo Effect," (presented by C.E. Sosolik.)

Leiden University Van Marum Seminar, Leiden, Netherlands, Febuary 2001, "Heavy Atom-Surface Scattering and the Search for the 'Flying' Kondo Effect," (presented by C.E. Sosolik.)

Contributed talk at the March Meeting of the American Physical Society, Seattle, WA, March 2001, "STM Investigation of Atom/Vacancy Formation During Direct Ion Deposition," (presented by J.M. Pomeroy.)

Contributed talk at the March Meeting of the American Physical Society, Seattle WA, March 2001, "Heavy Atom-Surface Scattering with Hyperthermal Energies," (presented by C.E. Sosolik.)

Materials Research Society Spring Meeting, San Francisco, CA, April 2001, "STM Investigation of Energetic Insertion During Direct Ion Beam Deposition," (presented by J.M. Pomeroy.)

Approximately 60 invited talks prior to reporting period (B.H. Cooper).

b) **Advisory functions.**

Invited member of Panel to define new directions and frontiers in "Surface Interactions with Photons, Electrons, Ions, Atoms, and Molecules" for the Department of Energy, Division of Chemical Sciences. Involved attending a Workshop on Atomic, Molecular, and Optical Physics, September 21-24 1997, Chantilly, VA and contributing to a written report. Contact – Dr. Joe Martinez.

Industrial Review and Workshop, University of Maryland Materials Research Science and Engineering Center, Invited Participant, College Park, MD, September 1997. Contact – Dr. Ellen Williams.

Search Committee for the U.S. Army Research Office, 1995, Research Triangle Park, NC. Contact – Dr. Robert Guenther, Director of the Physics Division at the Army Research Office.

Member of the Editorial Board of The Review of Scientific Instruments, 1993-96.

Member of the Executive Committee of the Instrumentation and Measurement Science Topical Group of the American Physical Society, 1994-97.

Member of the Organizing Committee of the Twelfth International Workshop on Inelastic Ion-Surface Collisions, 1996-99. Contacts – Drs. P. Nordlander and J.W. Rabalais.

Executive Committee of the Cornell Center for Materials Research, Representative of the College of Arts & Sciences, 1997-present. Contact—Dr. N.W. Ashcroft.

Executive Committee of the Division of Condensed Matter Physics of the American Physical Society, Member-At-Large, 1998.

Co-organizer of Symposium on "Real-Time Thin-Film Crystal Growth and Pattern Formation" at the 1998 Users Meeting of the Cornell High Energy Synchrotron Source. Contact—Dr. Sol Gruner.

Users Executive Committee for the Cornell High Energy Synchrotron Source, Vice Chair, 1998-. Contact—Dr. Sol Gruner.

Organizer of Symposium on "Ion-Surface Interactions" for the Fall 1999 MRS Meeting. Contact—Dr. Ellen Williams.

Co-hosted workshop on "Electron Tunneling" as part of the 1997 IAAY Conference at Cornell, "Exploring the Quantum World."

Gave lab tour to members of the Cornell Council. Contact—Dr. R.C. Richardson.

c) Transitions.

We have designed, in collaboration with Physicon Corporation, a beam line for producing mass- and energy-selected beam of hyperthermal energy ions. The beam energies range from a few eV to 10 keV. The species include metal, semiconductor, and reactive gas ions. Contact H. Von Zweck.

6) NEW DISCOVERIES, INVENTIONS, OR PATENT DISCLOSURES

New discoveries:

- Measured scaling exponent describing the separation of mounds during sputter-induced pattern formation on the Au(111) surface.
- Found preliminary evidence of a transition from mounded to smooth morphology evolution during sputtering of Au(111) controlled by the angle of incidence of the sputter beam.

Inventions:

- Ion beam optics for controlling space charge spreading during transport of hyperthermal energy ions.
- Hybrid Molecular Dynamics/Kinetic Monte Carlo code for simulating energetic beam deposition.

Patent disclosures:

None.

7) HONORS/AWARDS

Fellow of the American Physical Society, 1995 to 1999.

National Science Foundation Faculty Award for Women Scientists and Engineers, 1991-97.

8) REFERENCES

[1] J. Greene, S. Barnett, J. Sundgren, and A. Rockett, in *Ion Beam Assisted Film Growth*, ed. T. Itoh (Elsevier, Amsterdam, 1989), p. 101.

[2] S. Esch, M. Bott, T. Michely, and G. Comsa, Appl. Phys. Lett. **67**, 3209 (1995); M.Villarba and H. Jonsson, Surf. Sci. **324**, 35 (1995).

[3] E. Chason, et. al., Phys. Rev. Lett. **72**, 3040 (1004); T.M. Mayer, et. al., J. Appl. Phys. **76**, 1633 (1994); M. Ritter, etl al., Surf. Sci. **348**, 243 (1996); T. Michely and G. Comsa, Nucl. Instrum. Meth. B**82**, 207 (1993); S.J. Chey, et. al., Phys. Rev. B**52**, 16696 (1995).

[4] M.V. Ramana Murty, T. Curcic, A. Judy, B.H. Cooper, A.R. Woll, J.D. Brock, S. Kycia, and R.L. Headrick, X-Ray Scattering Study of the Surface Morphology of Au(111) During Ar+ Ion Irradiation, Phys. Rev. Lett. **80**, 4713 (1998).

[5] MRS Bulletin, Special Issue: Magnetism on a Microscopic Scale, **XX** No. 10 (1995); Physics Today, Special Issue: Magnetoelectronics **48**, No. 4 (1995).

[6] B. Poelsema, R. Kunkel, N. Nagel, A.F. Becker, G. Rosenfeld, L.K. Verheij, G. Comsa, Appl. Phys. A **53**, 369 (1991).

[7] J. Jacobsen, B.H. Cooper, and J.P. Sethna, Phys. Rev. B,**58** 15847 (1998).

[8] *Fractal Concepts in Crystal Growth*, A.-L. Barabasi and H.E. Stanley, Cambridge University Press, 1995.

[9] M.V. Ramana Murty, T. Curcic, A. Judy, B.H. Cooper, A.R. Woll, J.D. Brock, S. Kycia, and R.L. Headrick, *Real-Time X-Ray Scattering Study of Surface Dynamics on Au(111) During Ar^+ Ion Irradiation*, Mechanisms and Principles of Epitaxial Growth in Metallic Systems, 195 (1998)..

[10] T. Curcic – "*Thermal Smoothing of a Rough Au(111) Surface: An X-Ray Study,*" Cornell PhD Thesis (1998).

[11] M.V. Ramana Murty and B.H. Cooper, Phys. Rev. B **54**, 10377 (1996).

[12] M.V. Ramana Murty and B.H.Cooper, Surf. Sci., **415** 328 (1998).

[13] M.V. Ramana Murty and B.H.Cooper, Phys. Rev. B, **60** 16956 (1999).

[14] C.E. Carlston and G.D. Madson, Rev. Sci. Instr., **33**, no. 9, 905-911 (1962).

[15] Y.-W. Kim, I. Petrov, H. Ito, and J. Greene; J. Vac. Sci. Tech. A, **13(6)**, 2836-2842 (1995).

[16] T. Michely and C. Teichert, Phys. Rev. B, **50** 15, 11156 (1994).

[17] P. Stolze, J. Phys. Condens. Matter, **6,** 9495 (1994).